

Activity report of the European Crystallographic Association

April 2022 – March 2023



European Crystallographic Meeting in Versailles (ECM33)

Although the Covid-19 pandemic was not yet completely behind us in 2022, European crystallographers started to meet again in person, taking benefit of a relatively calm Covid period during summer. The scientific highlight of the European Crystallographic Association (ECA) in 2022 was the gathering of 805 delegates and 78 exhibitors at the 33th European Crystallographic Meeting from 23rd – 27th August 2022 in Versailles, France. The scientific program comprised a dense mixture of topics in 47 microsymbosia through all branches of crystallography. Two public lectures were devoted to the local French context: one on the life and work of René-Just Haüy, one of the founding fathers of modern crystallography who died 200 years ago in Paris, and the other one on the scientific aspects of the renovation of the Notre Dame cathedral in Paris that suffered a devastating fire in 2019.

The meeting also saw three ECA prizes awarded: the Perutz prize went to Professor Bill Clegg (Newcastle University, UK), the Kálmán prize to Professor Éric Collet (University of Rennes, France) and the Bertaut prize to Dr. Lukáš Gajdos (Institut Laue-Langevin, Grenoble, France). The 2021 Bertaut prize was awarded this year as well: Ellen Fogh from the EPFL in Lausanne was the lucky awardee, but received the prize at the International Conference on Neutron Scattering in Argentina.

In 2022, European crystallographers celebrated the foundation of the European Crystallographic Association 25 years ago in Lisbon, Portugal. It succeeded the European Crystallographic Committee (ECC) that was founded exactly 50 years ago in 1972 in Bordeaux, France, at the very first European Crystallographic Meeting. We had the pleasure to welcome in Versailles all past presidents of ECA except one, but also one of the founding fathers of ECC and ECA, Paul Beurskens (Nijmegen, the Netherlands) who, despite his 88 years, is still remarkably vivid. Paul and the past presidents, together with Bill Clegg representing ECA's senior crystallographers and Philipp Hans representing ECA's young crystallographers presented their views and highlights of European crystallography during a special ceremony.



From left to right: Marijana Đaković, Andreas Roodt, Hartmut Fuess, John Helliwell, Santiago Garcia-Granda, Claude Lecomte, Philipp Hans, Alessia Bacchi, Udo Heinemann, Bill Clegg, Paul Beurskens



Many delegates had dinner together during a magnificent boat trip on the Seine river, straight through the heart of Paris, underneath the Eiffel Tower and the Notre Dame cathedral.

ECA's webinars

European crystallographers continue to meet during ECA's monthly lunchtime webinars, a successful series of on-line seminars covering all sub-disciplines in crystallography and organized by ECA's young crystallographers. Ten lunch-time webinars took place from April 2022 until March 2023, only interrupted in August and September 2022:

- 7th April 2022. Nicole Benedek (USA) *Understanding the influence of the lattice on the functional properties of complex oxides: Physical mechanisms and crystal chemistry*
- 12th May 2022 Chiara Massera (Italy) *Turning "weakness" into strength: supramolecular interactions in crystals*
- 2nd June 2022 Holger Stark (Germany) *Atomic-resolution structure determination of proteins by cryo-EM: Where are the limits?*
- 7th July 2022 Alain Gibaud (France) *Probing nano-sized objects by (grazing-incidence) small angle scattering and coherent X-ray diffraction imaging*
- 6th October 2022 Gift Mehlana (Zimbabwe) *Metal-Organic Frameworks as Platforms for Hosting Molecular and Bio-Catalysts for Carbon Dioxide Hydrogenation*
- 3rd November 2022 Thomas A. White (Germany) *Real-time crystallographic data processing with streaming data*
- 1st December 2022. Regine Herbst-Irmer (Germany) *Twinning in Chemical Crystallography*
- 19th January 2023 Piero Macchi *Quantum crystallographic investigations of metal-metal bonded systems*
- 2nd February 2023 Henrik M. Rønnow (Switzerland) *Fundamentals of neutron scattering*
- 2nd February 2023 Jian-Rui Soh (Switzerland) *Recent advancement in magnetic neutron diffraction: detection of inversion-symmetry breaking local magneto-electric multipoles*
- 9th March 2023 Simona Galli (Italy) *Navigating within the pores of advanced porous materials: the power of powder diffraction*

Another series of webinars, the *Distinguished Lectures on Quantum Crystallography and Complementary Fields*, initiated by ECA's Special Interest Group 2 (Quantum Crystallography) and the IUCr commission on Quantum Crystallography continued as well: 7 webinars took place, usually with two lectures during the same webinar:

- 28th April 2022 Alessandro Genoni (France) *Development of Methods with a Strong Interplay between Quantum Chemistry and X-ray Diffraction Measurements*
- 28th April 2022 Johannes Neugebauer (Germany) *Electron Densities from Subsystem Density-Functional Theory*
- 19th May 2022 Christian Jelsch (France): *Charge Density & Intermolecular Interactions*
- 19th May 2022 Thomas Barend (Germany): *Watching Molecules at Work with Free-Electron Lasers*
- 29th September 2022 Bo Brummerstedt Iversen (Denmark) *Chemical bonding and local order*
- 29th September 29, 2022 Simon Billinge (USA) *Do materials have a genome, and if they do, what can we do with it?*
- 27th October 2022 Parthapratim Munshi (India) *On the Potency of Polymorphic Bioactive Molecules: A Quantum Crystallographic Perspective*
- 27th October 2022 Marcus A. Neumann (Germany) *Detecting and avoiding disappearing polymorph cases by crystal structure prediction*
- 1st December 2022 Paulina Dominiak (Poland) *Modelling electrostatic potential in electron diffraction studies*
- 1st December 2022 Richard Beanland (UK) *Exploring dynamical scattering using 'digital' large-angle convergent beam electron diffraction (D-LACBED) patterns*
- 1st December 2022 Lukas Palatinus (Czech Republic) *3D electron diffraction for charge density analysis: what are the challenges?*
- 12th January 2023 Jean-Michel Gillet (France) *Phase Space Quantum Crystallography: how about considering the other axis?*
- 12th January 2023 Katarzyna Pernal (Poland) *Reduced Functions and Descriptors for Accurate Electronic Structure Prediction and Understanding Chemical Bonding*
- 16th February 2023 Saulius Gražulis (Lithuania) *Open databases: what do we have, where are we going?*
- 16th February 2023 Julian Henn (Germany) *Global data quality metrics and data quality filter systems*

Work of the Executive Committee and decisions by the Council

ECA's executive committee continued working on different topics, at meetings in Zagreb (29th-30th April 2022), in Padova (17th-19th February 2023) and during two meetings in Versailles, but of course also very often remotely. Since the adoption of new statutes by the Council in 2021, we aim to obtain the charity – ANBI – status in the Netherlands (where ECA is registered) for two reasons: ECA is a non-profit organization working for the benefit of the community of European crystallographic science and should be recognized as such, but it will also put ECA on safe legal ground in terms of its charitable and tax status for the prizes and grants that are awarded every year. The procedure to acquire the ANBI status was started late February and is hoped to be achieved in the summer of 2023.

A new treasurer was elected during the Council Meeting in Versailles: Antonia Neels from EMPA and the University of Fribourg, Switzerland succeeding to Jacob Overgaard who decided to make a turning point in his career. We thank Jacob for serving ECA during four years. The Council also approved a bid from Nancy to organize the 9th European Crystallographic School in 2024, after that of Berlin in 2023 and the one which was held in Lisbon, Portugal, in July 2022.

ECA's Executive Committee Winter Meeting in Padova (17-19 February 2023), hosted by the ECM34 chair Gilberto Artioli, gave the committee the opportunity to visit Padova's brand new Congress Center where the 34th European Crystallographic Meeting will take place in 2024. Progress in the organization of future ECA events (ECM35, Lviv; ECS8, Berlin; ECS9, Nancy) have been discussed as well. A bid for the organization of a European Crystallography School in North Macedonia in 2025 will probably be submitted to ECA's Council for its meeting in September 2023.



The Executive Committee met in Padova from 17th to 19th February 2023. Some officers were not present physically. From left to right: Andy Maloney, Klaudia Hradil, Arie van der Lee, Marijana Đaković, Antonia Neels, Angela Altomare (IUCr representative), Consiglia Tedesco. Photo taken by Gilberto Artioli in front of the building of the Dipartimento di Geoscienze of the University of Padova

The Executive Committee continues to work on new web platforms on behalf of the communication of ECA's Special and General Interest Groups (SIGs and GIGs) which will be hopefully available before the 2023 Council Meeting of September. The Executive Committee will also submit a proposal to the Council for the creation of a SIG dedicated to crystallography in art and cultural heritage.

Another initiative is the creation of a new prize for *non-tenured* crystallographers to be financed from funds at Göttingen University resulting from industrial license fees for the SHELX programs. The Executive Committee will submit a proposal to the Council when it has decided on the guidelines for nominations for this new prize.

Work has been done by the Executive Committee to increase the attractiveness of the existing ECA prizes, Perutz, Kálmán and Bertaut. Discussions on how to achieve this have taken place at the Council Meeting in Versailles, but also with ECA's young crystallographers and board members of the Executive Committees of the American Crystallographic Association and the European Neutron Scattering Association. The Executive Committee has discussed and will draft new procedures and guidelines for the nominations for its prizes. Some changes need to be approved by the Council, since they require a change of the by-laws of the association.

The Executive Committee also discussed the possibility that ECA's European Crystallographic Schools offer ECTS credits to participants who have attended the school during its full duration and who have passed successfully a two-hours written examination at the last day of the school and have received a positive assessment of their practical work. ECTS points are only relevant for participants coming from a European university and acceptance of the credit points by the student's home university must be negotiated by the students themselves on the basis of the detailed School programme, the result of their examination and the assessment of their work by the School directors. The organisers of the school should negotiate the delivery of ECTS points with the University of the town where the School takes place.

The Executive Committee also exchanged views with Erhard Irmner (University of Göttingen) following a very fruitful discussion started in GIG03 by John Helliwell about a networking action on how to introduce crystallography related subjects in high-school programs in different countries.

Work is in progress to establish a *gender balance and equity statement* by ECA which should be taken into consideration for ECA's own events such as ECM and ECS, but also as a condition to receive financial support for non-ECA events. A proposal is being made by ECA's General Interest Group GIG3 and will be edited by the Executive Committee before discussion at the Council Meeting in September 2023.

Grants of ECA

One of the main reasons of ECA's existence is the financial support that ECA awards to young scientists for travelling to crystallography-related schools, workshops and congresses. We awarded last year 9 travel grants to young crystallographers for ECM33 in Versailles. We supported also financially 7 different meetings in 2022, of which 2 were pending from 2020, taking place only this year after two years of Covid-19 pandemic.

2022: Pending from 2020:

- Openlab of Crystallography, Initiative for Crystallography, Brazzaville (Congo), 11th to 22nd May 2022
- The Zurich School of Crystallography 2021 – Bring Your Own Crystals, University of Zurich, Zurich, Switzerland, 19th to 30th June 2022

2022:

- 56th Course of the International School of Crystallography "High Pressure Crystallography", Erice, Italy, 3rd to 11th June 2022
- 57th Course of the International School of Crystallography "Diffuse Scattering", Erice, Italy, 3rd to 11th June 2022
- 2nd International Charge Density Meeting (ICDM2), Aarhus, Denmark, 12th to 16th June 2022,
- 7th European Crystallographic School, ECS7, Lisbon, Portugal, 10th to 15th June 2022
- 24th Heart of Europe Bio-Crystallography Meeting (HEC24), Lipno – Dolní Vltavice, Czech Republic, 22th -24th September 2022

Initiatives in Africa

ECA continues to support the development of crystallography in Africa. The African Crystallographic Association (AfCA) was established in 2021; AfCA and ECA have decided that ECA's African National Members may remain ECA National Member as long as they wish.

ECA was represented by its secretary Andy Maloney at the 3rd African Conference on Crystallography which took place in Nairobi, Kenya, from 17-21 January 2023. ECA's National Member officer Delia Haynes was of course also present in Nairobi in her role as AfCA's Executive Committee president.

ECA members are also involved in the AFRAMED/Remote labs project led by its past-president Claude Lecomte who has initiated this exciting development aiming to train African crystallographers in the techniques of single-crystal diffraction in laboratories equipped with single-crystal diffractometers elsewhere and to give them the opportunity to run their own experiments by remote access to the diffractometer in the distant laboratory. This project was launched in Nancy, France, on August 31th, 2022.

Outlook

The next in-person large international crystallographic meeting will be the 26th IUCr Congress in Melbourne, Australia, in 2023. About 10 Australians were present at ECM33 in Versailles; hopefully we will see a lot of Europeans travelling in 2023 to Down Under! ECM34 will take place in Padova, Italy, from 26th-31th August 2024 and is immediately followed at the same venue by EPDIC18, the 18th European Powder Diffraction Conference: a truly good opportunity for all European crystallographers to meet!